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14. ABSTRACT

Significant progress has been attained in this area: we have developed an algorithm for automatic ansatz generation, and have demonstrated our overall algorithm by obtaining solutions involving tens of ansatz. An addition of Pade approximation has lead to results of machine precision in short computational times. In the last year's work, in particular, multiple scattering algorithms were developed which can compute high-order high frequency solution in O (1) operations for configurations giving rise to (a) multiple scattering of fields diffracted at shadow boundaries, as well as (b) multiple scattering withing single non-convex bodies. Very recent results include O (1) solvers for (c) three-dimensional problems which can evaluate in a couple of hours, and in single processors, scattering by objects much larger than the largest that could be tackled by other methods, even by means of large supercomputers. In detail, using our high-frequency method we have produced preliminary three-dimensional results for a spherical scatterer of radius a. In these preliminary examples we have demonstrated computational times that do not change significantly, with essentially

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Final Report

Oscar P. Bruno

April 2005

OBJECTIVES

* Development of high-order volumetric scattering solvers in three-d

* Development of high-order high-frequency solvers

* Development of a high-order geometry-description capability

* Parallelization of fast high-order methods previously developed

REPORT

FAST, HIGH ORDER VOLUMETRIC SCATTERERS

A suite of solvers for (penetrable) volumetric scattering problems was developed in collaboration with the PI's former PhD student McKay Hyde (now Assitant Professor at Rice's Applied and Compuatational Mathematics Department). This work was in fact the subject of McKay's PhD thesis, which can be obtained at http://www.acm.caltech.edu/~bruno/02hyde_thesis_print.pdf

These contributions have been documented in three publications by Bruno and Hyde: two in the Journal of Computational Physics and one in SIAM Journal on Numerical Analysis, as listed in the publication section below.

In addition to this work, and in collaboration with McKay Hyde and long time collaborator Prof. F. Reitich we have developed a "thin volume scattering solver". This algorithm complements the work mentioned above: by splitting a general volume into a thin boundary volume and a large but smooth inner volume, the combined solver is the first one to provide high order convergence for volumetric scattering problems. This work is still in preparation.

HIGH FREQUENCY SOLVERS

Significant progress has been attained in this area: we have developed an algorithm for automatic ansatz generation, and have demonstrated our overall algorithm by obtaining solutions involving tens of ansatz. An addition of Pade approximation has lead to results of machine precision in short computational times. In the last year's work, in particular, multiple scattering algorithms were developed which can compute high-order high frequency solution in O(1) operations for configurations giving rise to (a) multiple scattering of fields diffracted at shadow boundaries, as well as (b) multiple scattering withing single non-convex bodies. Very recent results include O(1) solvers for (c) three-dimensional problems which can evaluate in a couple of hours, and in single processors, scattering by objects much larger than the largest that could be tackled by other methods, even by means of large supercomputers. In detail, using our high-frequency method we have produced preliminary three-dimensional results for a spherical scatterer of radius a. In these preliminary examples we have demonstrated computational times that do not change significantly, with essentially fixed accuracies, when the frequency increases. For example, we have obtained results for $ka=800$ up to $ka=3200$ with less than 5% error in a 200 minute computational time in a single 1.5 GHz PC processor. This computing time is several orders of magnitude smaller than the computational time required by other state of the art algorithms. For reference, results produced by means of the Fast Multipole Method (FISC), the solution for a 120λ sphere required 9.6 million unknowns and 14.5 hours of CPU time on a 32 processor SGI Origin 2000, leading to an RMS Error of 4.6%. Although this is only a rough comparison (since the FISC results were obtained for the vector Maxwell system and our preliminary results were obtained for the scalar Helmholtz equation), our solutions were obtained using 4096 unknowns in about three hours on a single processor 1.5 GHz PC, and for much larger frequencies.

HIGH-ORDER GEOMETRY-DESCRIPTION

The problem of producing smooth representations from a triangulation has been considered often in recent years. Previous methods have sought to utilize piece-wise polynomial approximations, and, under certain asumptions concerning regularity of a given triangulation, have provided representations with continuous derivatives of first order. Higher order differentiability has not been produced by any other means as yet, and the prospects for the feasibility of such extensions do not seem favorable: it appears that piecewise polynomial approximations may not be helpful in our context. Our approach to high order geometry representation is based on use of Fourier series for certain periodic functions associated with the given surface. As a result of our efforts during the last year in this area, our methods of surface representation have been extended and improved, giving rise to improved rendering of complex features; for example, air intakes are produced through a combination of one- and two-dimensional Fourier representations.

EDGES AND OPEN SURFACES

A new concept of Canonical integrals has given rise to significant improvements in the treatment of integral equations at edges, wire geometries, high-frequency solvers in three dimensions, and open surfaces (plates). In addition, use of new "edge-integral-asymptotics" has allowed extension of the Canonical integral method to fully electromagnetic problems.

PARALLELIZATION

Parallelization of existing high-order methods has proceeded according to schedule; currently a fully parallel solver for the Maxwell equations is implemented. The last issue that remains for completion of this task is to improve the parallelization of the FFTs used by the equivalent source acceleration algorithm.

ARCHIVAL PUBLICATIONS

"Explicit and stable evolution of the generalized nonlinear Schroedinger equation", D. Amundsen and O. Bruno, submitted to IEEE Journal of Lightwave Technology.

"Pade time-stepping (PTS): a stable explicit scheme", D. Amundsen and O. Bruno, submitted to SIAM J. Sci. Comput.

"On the O(1) solution of multiple-scattering problems", C. Geuzaine, O. Bruno, and F. Reitich. To appear in IEEE Trans. Magn., 2005.

"One-dimensional inverse scattering problem for optical coherence tomography" , O. Bruno and J. Chaubell; To appear in Inverse Problems, 2005

"Higher-order Fourier approximation in scattering by two-dimensional, inhomogeneous media", O. Bruno and M. Hyde; To appear in SIAM J. Numer. Anal. (April 2005)

"A new high-order high-frequency integral equation method for the solution of scattering problems I: Single-scattering configurations", O. Bruno, C. Geuzaine, and F. Reitich, The 20th Annual Review of Progress in Applied Computational Electromagnetics (ACES 2004), April 19-23, 2004 - Syracuse, NY

"A new high-order high-frequency integral equation method for the solution of scattering problems II: Multiple-scattering configurations", O. Bruno, C. Geuzaine, and F. Reitich, The 20th Annual Review of Progress in Applied Computational Electromagnetics (ACES 2004), April 19-23, 2004 - Syracuse, NY

"An efficient, preconditioned, high-order solver for scattering by two-dimensional, inhomogeneous media", O. Bruno and M. Hyde; J. Comput. Phys. 200 670--694 (2004).

"A Fast, High-Order Method for Scattering by Penetrable Bodies in Three Dimensions", M. Hyde and O. Bruno; J. Comput. Phys. 202 236--261 (2005).

"Inverse scattering problem for optical coherence tomography", O. Bruno and J. Chaubell; Optics Letters. 28, 2049-2051 (2003).

"Wave scattering by inhomogeneous media: efficient algorithms and applications", O. Bruno; Physica B 338, 67-73, (2003).

"A fast high-order solver for problems of scattering by heterogeneous bodies", O. Bruno and A. Sei; IEEE Trans. Antenn. Propag. 51, pp. 3142-3154 (2003).

"Fast, high-order, high-frequency integral methods for computational acoustics and electromagnetics", O. Bruno, Topics in Computational Wave Propagation: Direct and Inverse Problems, Lecture notes in computational science and engineering, 31 43-82. Springer Verlag, 2003.

"A fast algorithm for the simulation of polycrystalline misfits II: martensitic transformations in three space dimensions", G. Goldsztein and O. Bruno; Proc. Roy. Soc. London, 03PA0117/1-03PA0117/18 (2004).

HONORS/AWARDS

PI will be/was plenary speaker at the conferences

"Future Directions in Applied Mathematics-International Conference on the occasion of Jean-Claude Nedelec's 60th Birthday" (Ecole Polytechnique, Paris, France.) June 18-21, 2003.

"Third International Conference on Boundary Integral Methods: Theory and Applications" (University of Reading, London Mathematical Society). 14-18 September 2004.

"XIV Congress on Numerical Methods and their Applications" (Bariloche, Argentina.) 8-11 November 2004.

"7th International Conference on Mathematical and Numerical Aspects of Wave Propagation" (WAVES'05, Brown University, Rhode Island.) June 20-24, 2005.